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Numerical experiments for phase change problems

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1. Problems and existence–uniqueness results.

We consider the following coupled system of nonlinear parabolic PDEs:

$$
(P_{\nu\kappa})\begin{cases} (u+w)_t - \Delta u = f(t,x) & \text{in } Q := (0,+\infty)\times\Omega, \\ \nu w_t - \kappa\Delta w + \beta(w) + g(w) \ni u & \text{in } Q, \\ \dfrac{\partial u}{\partial n} + n_0 u = h(t,x) & \text{on } \Sigma := (0,+\infty)\times\Gamma, \\ \dfrac{\partial w}{\partial n} = 0 & \text{on } \Sigma, \\ u(0,\cdot) = u_0, \quad w(0,\cdot) = w_0 & \text{in } \Omega. \end{cases}
$$

Here Ω is a bounded domain in $\mathbf{R}^N$ $(1 \le N \le 3)$ with smooth boundary $\Gamma := \partial\Omega$. Both ν and κ are non-negative parameters.

This system is proposed as a thermodynamical phase–field model with constraint. In this model, u is the temperature and w is a non–conserved order parameter which indicates physical state of the material. This system can be derived along the thermodynamical approach by Penrose–Fife [10] from the following free energy functional

$$
F_\Omega(u,w) = \int_\Omega \{\frac{\kappa}{2}|\nabla w|^2 + \hat{\beta}(w) + \hat{g}(w) - uw\}dx
$$

where $\hat{\beta}$ is a proper l.s.c. convex function on $\mathbf{R}$ with subdifferential $\beta = \partial\hat{\beta}$ in $\mathbf{R}$ and $\hat{g}$ is a primitive of g.

We discuss problem $(P_{\nu\kappa})$ under the following assumptions.

(A1) β is a maximal monotone graph in $\mathbf{R}\times\mathbf{R}$ such that $\overline{D(\beta)} = [\sigma_*, \sigma^*]$ for some constants σ_*, σ^* with $-\infty < \sigma_* < \sigma^* < +\infty$.

(A2) g is a Lipschitz continuous function in $\mathbf{R}$.

(A3) $f \in L^2_{loc}(\mathbf{R}_+; L^2(\Omega))$.

(A4) $h \in W^{1,2}_{loc}(\mathbf{R}_+; L^2(\Gamma)) \cap L^\infty(\mathbf{R}_+; L^\infty(\Gamma))$.

(A5) n_0 is a positive constant.

(A6) $u_0, w_0 \in L^2(\Omega)$ with $\sigma_* \le w_0 \le \sigma^*$ a.e. in Ω.

We denote by $(\cdot,\cdot)$ the standard inner product in $L^2(\Omega)$, by $H^1(\Omega)^*$ the dual space of $H^1(\Omega)$, and by $\langle\cdot,\cdot\rangle$ the duality pairing between $H^1(\Omega)^*$ and $H^1(\Omega)$. Also, we denote by $C_w([0,T]; L^2(\Omega))$ the space of all weakly continuous functions from $[0,T]$ into $L^2(\Omega)$, and mean by " $v_n \to v$ in $C_w([0,T]; L^2(\Omega))$ as $n \to +\infty$ " that $(v_n(t) - v(t), z) \to 0$ uniformly in $t \in [0,T]$ for each $z \in L^2(\Omega)$.

We now introduce the weak formulation for problem $(P_{\nu\kappa})$.

Definition 1.1 A couple of functions $u := u_{\nu\kappa} : \mathbf{R}_+ \to H^1(\Omega)^*$ and $w := w_{\nu\kappa} : \mathbf{R}_+ \to L^2(\Omega)$ is called a (weak) solution of $(P_{\nu\kappa})$, if the following conditions $(\mathrm{N1})_i$–$(\mathrm{N3})_i$, $(i = 1,2,3)$ are fulfilled for any finite $T > 0$.
(i) If $\nu > 0$ and $\kappa > 0$, then

$(\mathrm{N1})_1$ $u \in C([0,T]; H^1(\Omega)^*) \cap W^{1,2}_{loc}((0,T]; H^1(\Omega)^*) \cap L^2(0,T; L^2(\Omega)) \cap L^2_{loc}((0,T]; H^1(\Omega))$,
$w \in C([0,T]; L^2(\Omega)) \cap W^{1,2}_{loc}((0,T]; L^2(\Omega)) \cap L^2(0,T; H^1(\Omega))$,
and $\hat\beta(w) \in L^1(0,T; L^1(\Omega))$;

$(\mathrm{N2})_1$ The variational equality

$$\langle u'(t) + w'(t), z\rangle + \int_\Omega \nabla u(t)\cdot\nabla z dx + \int_\Gamma (n_0 u(t) - h(t)) z d\Gamma = (f(t), z) \qquad (1.1)$$

holds for all $z \in H^1(\Omega)$ and a.e. $t \in [0,T]$, and $u(0) = u_0$;

$(\mathrm{N3})_1$ there exists $\xi \in L^2_{loc}((0,T]; L^2(\Omega))$ such that $\xi \in \beta(w)$ a.e. in $Q_T := (0,T)\times\Omega$ and

$$\nu(w'(t), z) + \kappa\int_\Omega \nabla w(t)\cdot\nabla z dx + (\xi(t), z) + (g(w(t)), z) = (u(t), z) \qquad (1.2)$$

for all $z \in H^1(\Omega)$ and a.e. $t \in [0,T]$, and $w(0) = w_0$.

(ii) If $\nu > 0$ and $\kappa = 0$, then

$(\mathrm{N1})_2$ $u \in C([0,T]; H^1(\Omega)^*) \cap W^{1,2}_{loc}((0,T]; H^1(\Omega)^*) \cap L^2(0,T; L^2(\Omega)) \cap L^2_{loc}((0,T]; H^1(\Omega))$,
$w \in C([0,T]; L^2(\Omega)) \cap W^{1,2}_{loc}((0,T]; L^2(\Omega))$, and $\hat\beta(w) \in L^1(0,T; L^1(\Omega))$;

$(\mathrm{N2})_2$ $= (\mathrm{N2})_1$;

$(\mathrm{N}3)_2$ there exists $\xi \in L^2_{loc}((0,T];L^2(\Omega))$ such that $\xi \in \beta(w)$ a.e. in Q_T and

$$\nu(w'(t),z)+(\xi(t),z)+(g(w(t)),z)=(u(t),z)$$

for all $z \in L^2(\Omega)$ and a.e. $t \in [0,T]$, and $w(0)=w_0$.

(iii) If $\nu = 0$ and $\kappa > 0$, then

$(\mathrm{N}1)_3$ $u \in L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;H^1(\Omega))$, $w \in L^\infty(0,T;H^1(\Omega))$, $u+w \in C_w([0,T];L^2(\Omega))$, $(u+w)_t \in L^2(0,T;H^1(\Omega)^*)$, and $\hat{\beta}(w) \in L^1(0,T;L^1(\Omega))$;

$(\mathrm{N}2)_3$ $= (\mathrm{N}2)_1$.

$(\mathrm{N}3)_3$ there exists $\xi \in L^2_{loc}((0,T];L^2(\Omega))$ such that $\xi \in \beta(w)$ a.e. in Q_T and

$$\kappa\int_\Omega \nabla w(t)\cdot\nabla z dx+(\xi(t),z)+(g(w(t)),z)=(u(t),z)$$

for all $z \in H^1(\Omega)$ and a.e. $t \in [0,T]$, and $w(0)=w_0$.

In the sequel, we denote by $\{u_{\nu\kappa}, w_{\nu\kappa}\}$ a solution of $(P_{\nu\kappa})$ in the sense of Definition 1.1.

In each case, an existence and uniqueness result is given in the following theorem.

Theorem 1.1 *Suppose (A1)–(A6) hold. Let T be any finite positive real number and both parameters ν and κ be non-negative. Then:*
(i) (cf.[1,4,7,9]) If $\nu > 0$ and $\kappa > 0$, then
problem $(P_{\nu\kappa})$ has one and only one solution $\{u_{\nu\kappa}, w_{\nu\kappa}\}$ on $[0,T]$.
(ii) (cf.[2,11]) If $\nu > 0$ and $\kappa = 0$, then
problem $(P_{\nu 0})$ has one and only one solution $\{u_{\nu 0}, w_{\nu 0}\}$ on $[0,T]$.
(iii) Let $\nu = 0$ and $\kappa > 0$, and further suppose that

$$(g(w_1)-g(w_2))(w_1-w_2)+(1-c_0)|w_1-w_2|^2 \geq 0$$

for all $w_1, w_2 \in \mathbf{R}$, where c_0 is a positive constant. Then problem $(P_{0\kappa})$ has one and only one solution $\{u_{0\kappa}, w_{0\kappa}\}$ on $[0,T]$.

For a detailed proof of Theorem 1.1 (iii), see a forthcoming paper of Sato, Kenmochi and the author [12].

2. Asymptotic behavior as ν or $\kappa \to 0$.

In this section, we give some numerical experiments concerning the asymptotic behavior of the order parameter $w_{\nu\kappa}$ as $\nu \searrow 0$ or $\kappa \searrow 0$, based upon the following theorem.

Theorem 2.1 *Let T be any positive finite number and suppose that (A1)–(A6) hold.*
(i) (cf.[2]) Let ν be a positive number. Then

$$u_{\nu\kappa} \to u_{\nu 0},\ w_{\nu\kappa} \to w_{\nu 0} \text{ in } C([0,T];L^2(\Omega)) \text{ as } \kappa \to 0.$$

(ii) Let κ be a positive number. Then

$$\begin{array}{ll} u_{\nu\kappa} \rightharpoonup u_{0\kappa} & \textit{weakly in } L^2(0,T;H^1(\Omega)) \textit{ as } \nu \to 0, \\ w_{\nu\kappa} \rightharpoonup w_{0\kappa} & \textit{weakly* in } L^\infty(0,T;H^1(\Omega)) \textit{ as } \nu \to 0, \\ u_{\nu\kappa} + w_{\nu\kappa} \to u_{0\kappa} + w_{0\kappa} & \textit{in } L^2(0,T;L^2(\Omega)) \cap C_w([0,T];L^2(\Omega)) \textit{ as } \nu \to 0. \end{array}$$

Numerical experiments are tried under the following situation (AS):

$$(AS) \begin{cases} \Omega \text{ is an interval } (0,L) \text{ in } \mathbf{R}, \\ g(w) = w^3 - w, \\ \beta \text{ is the subdifferential of the indicator function of the interval } [-0.5, 0.5], \\ n_0 \equiv 1, \\ h(x) \equiv l_0 \text{ for every } x \in \Omega, \text{ where } l_0 \text{ is a constant in } [-5,5]. \end{cases}$$

Experiment 2.1 (cf.Fig.2.1) In addition to (AS), suppose that $\nu = 1, l_0 = 0$ and $f \equiv 0$. Fixing initial data u_0, w_0, let κ tend to 0. Fig.2.1 includes four graphs of the function $w_{\nu\kappa}(T,\cdot)$ on the space interval $(0,L)$, which correspond to $\kappa = 0.1, 0.05, 0.01$ and 0, respectively. In each figure, there are two flat parts and a smooth curve between them. The upper (resp. lower) flat part is of pure liquid (resp. solid) phase and the smooth curve is the interface of liquid and solid.

We observe from these figures that the slope of the interface becomes gradually steep as κ goes to 0, and when $\kappa = 0$, the graph of $w_{\nu 0}(T,\cdot)$ is a step function on $(0,L)$.

Experiment 2.2 (cf.Fig.2.2) In addition to (AS), suppose now that $\kappa = 0.05, l_0 = 0$ and $f \equiv 0$. Fixing initial data u_0, w_0, let ν tend to 0. Fig.2.2 includes four graphs of the functions $w_{\nu\kappa}(t, \frac{3}{4}L)$ with respect to time $t \in [0,T]$, which correspond to $\nu = 1, 0.5, 0.05$ and 0, respectively.

We observe from these figures that the convergence of $w_{\nu\kappa}(t, \frac{3}{4}L)$ with respect to time becomes gradually fast as ν goes to 0.

3. Asymptotic behavior as $t \to +\infty$.

The steady–state problems, referred as (P^∞) in any case, are described as one of the following two systems.

(i) When $\kappa > 0$, (P^∞) is formulated by

$$\begin{cases} -\Delta u^\infty = f^\infty & \text{in } \Omega, \\ -\kappa \Delta w^\infty + \beta(w^\infty) + g(w^\infty) \ni u^\infty & \text{in } \Omega, \\ \dfrac{\partial u^\infty}{\partial n} + n_0 u^\infty = h^\infty & \text{on } \Gamma, \\ \dfrac{\partial w^\infty}{\partial n} = 0 & \text{on } \Gamma. \end{cases}$$

(ii) When $\kappa = 0$, (P^∞) is formulated by

$$\begin{cases} -\Delta u^\infty = f^\infty & \text{in } \Omega, \\ \beta(w^\infty) + g(w^\infty) \ni u^\infty & \text{in } \Omega, \\ \dfrac{\partial u^\infty}{\partial n} + n_0 u^\infty = h^\infty & \text{on } \Gamma. \end{cases}$$

Here $f^\infty \in L^2(\Omega)$ and $h^\infty \in L^2(\Gamma)$ are such that

$$f - f^\infty \in L^2(\mathbf{R}_+; L^2(\Omega)),\ h - h^\infty \in L^2(\mathbf{R}_+; L^2(\Gamma)). \tag{3.1}$$

It should be noted that the elliptic system

$$-\Delta u^\infty = f^\infty \text{ in } \Omega, \quad \frac{\partial u^\infty}{\partial n} + n_0 u^\infty = h^\infty \text{ on } \Gamma$$

dose not include w^∞, so it can be solved independently and the solution $u^\infty \in H^1(\Omega)$ is characterized in the variational sense by

$$\int_\Omega \nabla u^\infty \cdot \nabla z dx + \int_\Gamma (n_0 u^\infty - h^\infty) z d\Gamma = (f^\infty, z) \quad \text{for all } z \in H^1(\Omega). \tag{3.2}$$

Therefore, with the solution u^∞ of (3.2), if $\kappa > 0$, then the steady–state problem (P^∞) is formulated as an elliptic variational problem

$$(EP) \begin{cases} v \in H^1(\Omega); \\ \kappa \int_\Omega \nabla v \cdot \nabla z dx + \int_\Omega (\xi + g(v) - u^\infty) z dx = 0 \text{ for all } z \in H^1(\Omega), \\ \text{where } \xi \text{ is a function in } L^2(\Omega) \text{ with } \xi \in \beta(v) \text{ a.e. in } \Omega. \end{cases}$$

Also, if $\kappa = 0$, then (P^∞) is formulated as an algebraic relation on Ω

$$(AP) \begin{cases} v \in L^2(\Omega); \\ \beta(v(x)) + g(v(x)) \ni u^\infty(x) \quad \text{for a.e. } x \in \Omega. \end{cases}$$

Large time behavior of the solution $\{u_{\nu\kappa}, w_{\nu\kappa}\}$ of our problems are stated in the following theorems.

Theorem 3.1 *(cf.[6]) Suppose that ν and κ are positive, conditions (A1)–(A6) and (3.1) hold. Then:*
(1) $u_{\nu\kappa}(t) \rightharpoonup u^\infty$ weakly in $H^1(\Omega)$ as $t \to +\infty$, where u^∞ is the solution of (3.2).
(2) $w_{\nu\kappa}(t)$ does not converge, in general, as $t \to +\infty$. Consider the ω–limit set

$$\omega(u_0, w_0) := \{v \in H^1(\Omega);\ w_{\nu\kappa}(t_n) \to v \text{ in } H^1(\Omega) \text{ for some } t_n \text{ with } t_n \to +\infty\}. \tag{3.3}$$

Then:

(a) $\omega(u_0, w_0)$ *is non-empty, compact and connected in* $H^1(\Omega)$.
(b) Any function $v \in \omega(u_0, w_0)$ *is a solution of problem (EP).*

When $\kappa = 0$ and $\nu > 0$, the large time behavior of the order parameter w is quite different from the case of $\kappa > 0$ and $\nu > 0$, as the following theorem shows.

Theorem 3.2 *(cf.[11]) Suppose that* ν *is positive,* $\kappa = 0$, *conditions (A1)–(A6) and (3.1) hold. Further suppose that for each* $p \in \mathbf{R}$, *the (algebraic) inclusion*

$$\beta(r) + g(r) \ni p$$

has a finite number of solutions $r \in \overline{D(\beta)}$. *Then:*
(1) $u_{\nu 0}(t) \rightharpoonup u^\infty$ *weakly in* $H^1(\Omega)$ *as* $t \to +\infty$, *where* u^∞ *is the solution of (3.2).*
(2) *There exists a function* $w^\infty \in L^\infty(\Omega)$ *such that*

$$\beta(w^\infty(x)) + g(w^\infty(x)) \ni u^\infty(x) \text{ for a.e. } x \in \Omega,$$

and

$$w_{\nu 0}(t) \to w^\infty \text{ a.e. } x \in \Omega \text{ as } t \to +\infty.$$

When $\kappa > 0$ and $\nu = 0$, the large time behavior of the order parameter w is rather similar to that of the case when $\kappa > 0$ and $\nu > 0$.

Theorem 3.3 *Suppose that* $\nu = 0$ *and* κ *is positive, conditions (A1)–(A6) and (3.1) hold. Then:*
(1) $u_{0\kappa}(t) \rightharpoonup u^\infty$ *weakly in* $L^2(\Omega)$ *as* $t \to +\infty$, *where* u^∞ *is the solution of (3.2).*
(2) $w_{0\kappa}(t)$ *does not converge, in general. Consider the* ω*-limit set* $\omega(u_0, w_0)$ *defined by (3.3).*
Then:
(a) $\omega(u_0, w_0)$ *is non-empty in* $H^1(\Omega)$, *compact and connected in* $L^2(\Omega)$.
(b) Any function $v \in \omega(u_0, w_0)$ *is a solution of problem (EP).*

Now we give some numerical experiments of the asymptotic behavior of the order parameter as time goes to $+\infty$, based on the above theorems.

In our numerical experiments suppose that

$$f^\infty \equiv 0, \quad \text{and} \quad h^\infty \equiv l_0, \tag{3.4}$$

so

$$u^\infty \text{ is a constant } \frac{l_0}{n_0}.$$

Fig.3.1 shows how to look at our numerical computations. Also, the final time is big enough, so it can be numerically considered as $+\infty$.

Experiment 3.1 (cf.Fig.3.2–3.4) In addition to (AS) suppose that (3.4) holds and $\nu > 0, \kappa > 0$ are fixed. First of all we give three experiments in which the order parameter converges as $t \to +\infty$.

(1) Suppose $l_0 = 0$ and the initial datum w_0 is a step function. In this case, $u^\infty = \frac{l_0}{n_0} \equiv 0$, which is the phase transition temperature. Fig.3.2 shows that $w(t,\cdot)$ converges as $t \to +\infty$, despite the temperature u behaves near 0 for large time. Moreover, it shows that the limit of w at $t = +\infty$ is smooth in space, despite the initial datum is not smooth.

(2) Suppose $l_0 = -5$ and w_0 is a step function. The boundary datum $l_0 = -5$ keeps the temperature u very low (lower than the phase transition temperature). Fig.3.3 shows everywhere is of pure solid after a certain finite time. To the contrary, if the temperature is controlled to be very high, everywhere might be of pure liquid after a certain finite time.

(3) Suppose $l_0 = 0$ again, and w_0 is a smooth function. Fig.3.4 shows that the limit $w(t,\cdot)$ (as $t \to +\infty$) is quite similar to that in Fig.3.2, although the initial data are quite different from each other.

Experiment 3.2 (cf.Fig.3.5) In addition to (AS), suppose that (3.4) holds, $\kappa = \nu = 1$ and $l_0 = 0$ (hence $u^\infty \equiv 0$). Furthermore, $f = f(t,x)$ is a certain function in $L^2(\mathbf{R}_+; L^2(\Omega))$. Fig.3.5 shows that the pure liquid region ($= \{x \in (0,L); w(t,x) = 0.5\}$) oscillates horizontally forever, and the oscillation amplitude never deduce to 0 as $t \to +\infty$. But the oscillation speed becomes gradually slow as $t \to +\infty$. This means that the ω–limit set $\omega(u_0, w_0)$ of the order parameter w contains a continuum of steady–state solutions.

Such a kind of non–standard behavior of the order parameter w that was obtained in Experiment 3.2 may be caused by the terms

$$-\kappa\Delta w \quad \text{and} \quad \beta(w).$$

In fact, without $\beta(w)$, ω–limit set $\omega(u_0, w_0)$ is a singleton, that is, the order parameter w converges as time goes to $+\infty$ (cf.[5]). Also, without $-\kappa\Delta w$, namely $\kappa = 0$, as we discussed in Theorem 3.2, the order parameter w converges as $t \to +\infty$, although the cardinal number of all steady–state solutions is continuum.

Next we give some numerical experiments based on Theorem 3.2.

Experiment 3.3 (cf.Fig.3.6–3.8) In addition to (AS), suppose that (3.4) holds, $\nu > 0$ is fixed and $\kappa = 0$.

(1) Further suppose $l_0 = 0$ and the initial datum w_0 is a step function with three steps. Then Fig.3.6 shows that the limit of $w(t,\cdot)$ (as $t \to +\infty$) is a step function with two steps. This means that at $t = +\infty$ there are pure liquid region, pure solid region and their interface which is just one point.

(2) Suppose $l_0 = -5$ and w_0 is a step function. Then Fig.3.7 shows everywhere is of pure solid after a certain finite time, since the temperature u is kept very low.

(3) Suppose $l_0 = 0$ and w_0 is a smooth. Then Fig.3.8 shows that the limit of $w(t,\cdot)$ as $t \to +\infty$ is again a step function, even if w_0 is smooth.

Finally we give some numerical experiments, based on Theorem 3.3, which are similar to those as in Experiments 3.1 and 3.2.

Experiment 3.4 (cf.Fig.3.9–3.11) In addition to (AS), suppose that (3.4) holds, $\nu = 0$ and $\kappa > 0$ is fixed. We give two experiments in which the order parameter w converges as $t \to +\infty$.

(1) Further suppose $l_0 = 0$ and the initial datum w_0 is a step function. Then Fig.3.9 shows that $w(t, \cdot)$ converges as $t \to +\infty$ and the limit is smooth in space.

(2) Suppose $l_0 = -5$ and w_0 is a step function. Then, Fig.3.10 shows everywhere is of pure solid after a certain finite time.

(3) Suppose $l_0 = 0$. Then, for similar functions w_0 and f as in Experiment 3.2, the order parameter $w(t, \cdot)$ oscillates horizontally forever, and the ω–limit set contains a continuum of steady–state solutions.

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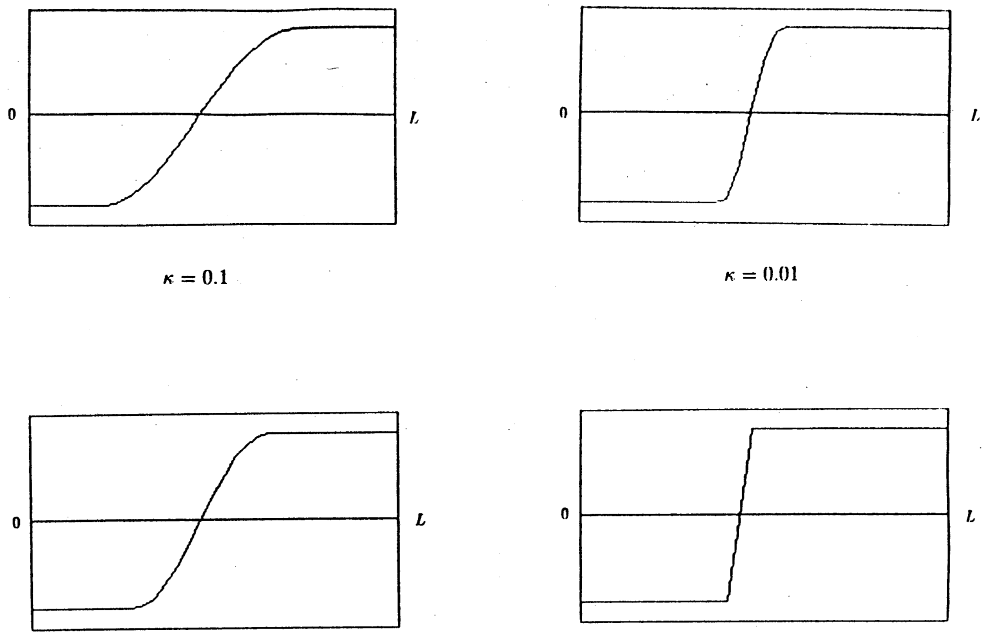
$t = T$

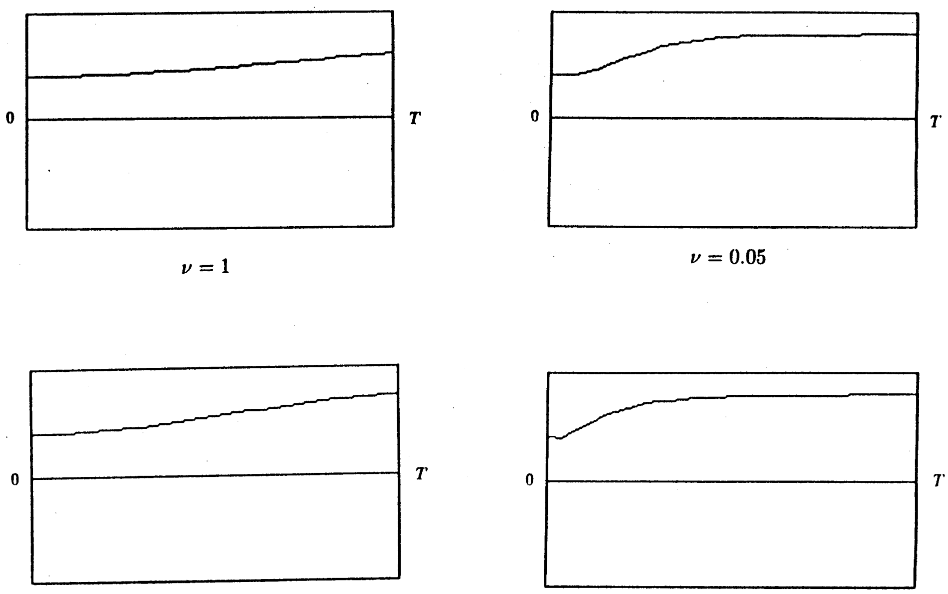


$\kappa = 0.1$ $\kappa = 0.01$

$\kappa = 0.05$ $\kappa = 0$

(Fig.2.1)

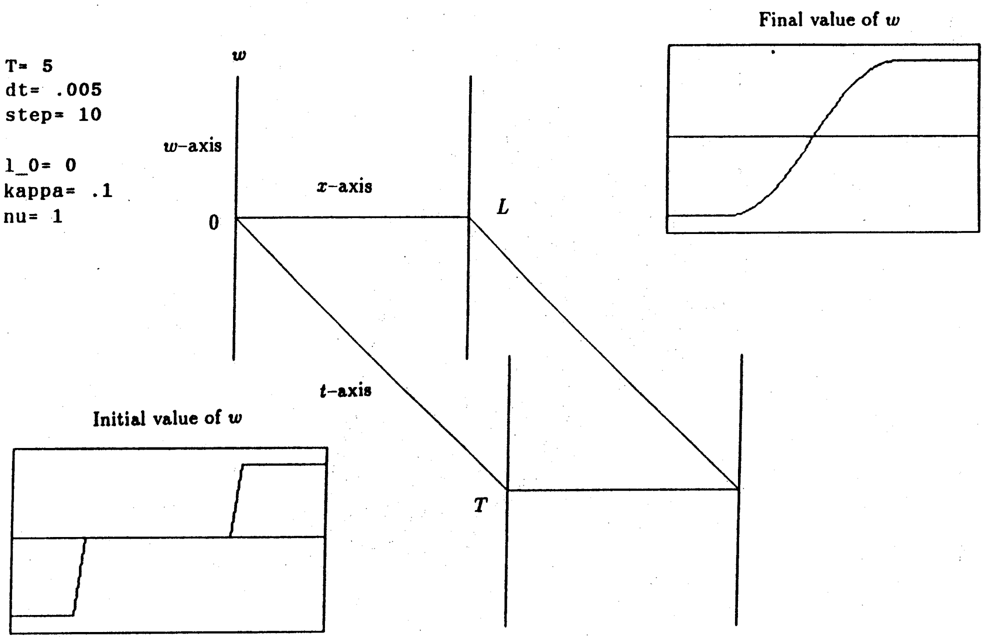
$x = \frac{3}{4}L$



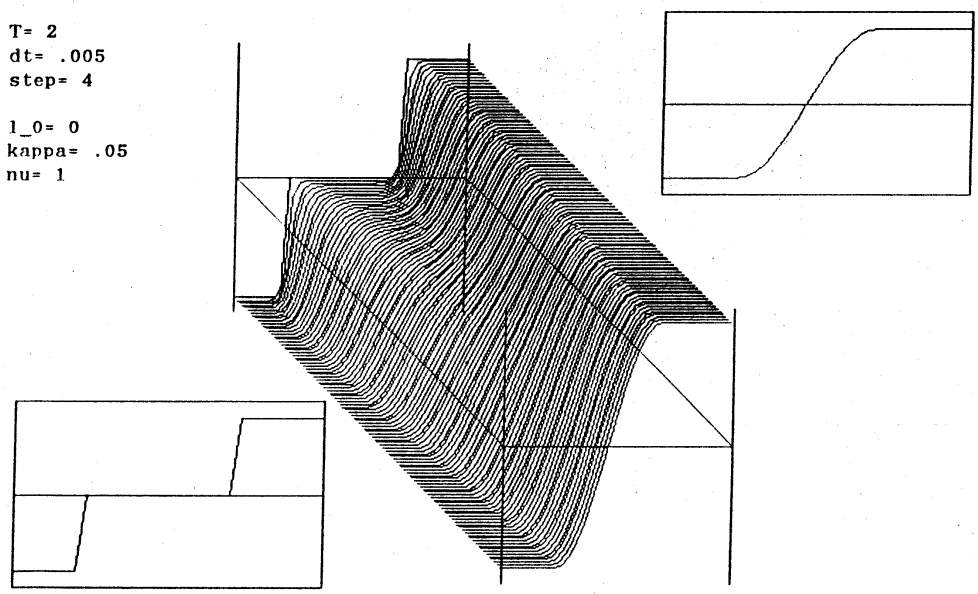
$\nu = 1$ $\nu = 0.05$

$\nu = 0.5$ $\nu = 0$

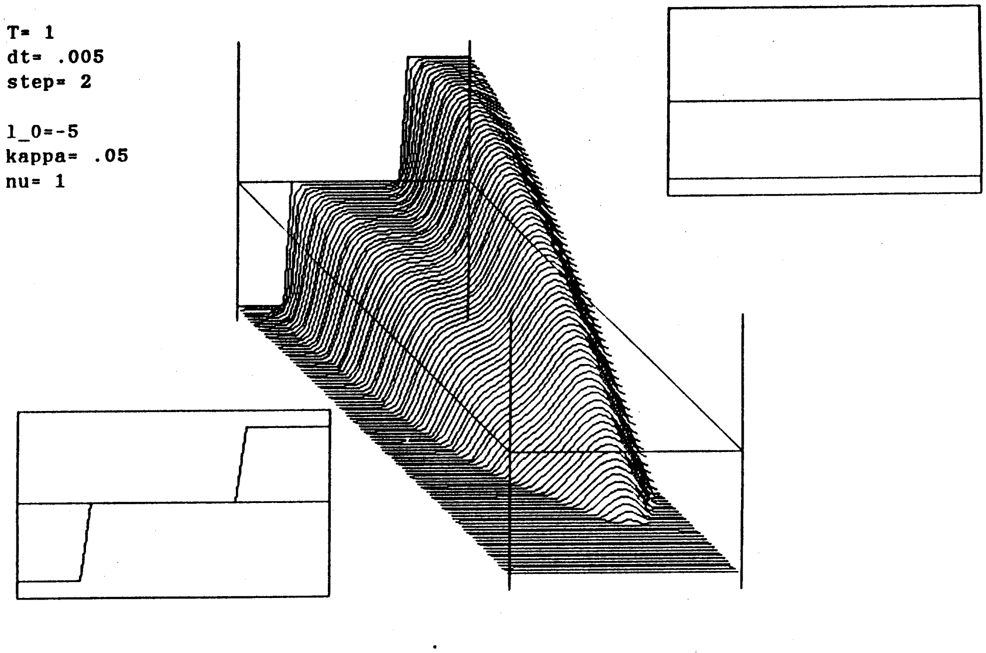
(Fig.2.2)


T= 5
dt= .005
step= 10
l_0= 0
kappa= .1
nu= 1
w
w-axis
x-axis
0
L
t-axis
T
Final value of w
Initial value of w

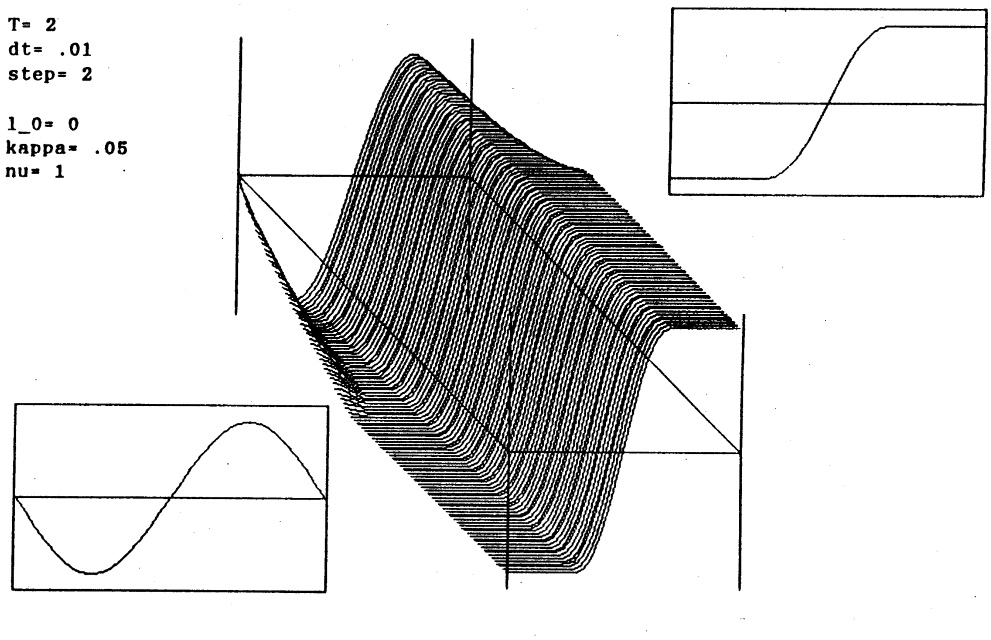
(Fig.3.1)


T= 2
dt= .005
step= 4
l_0= 0
kappa= .05
nu= 1

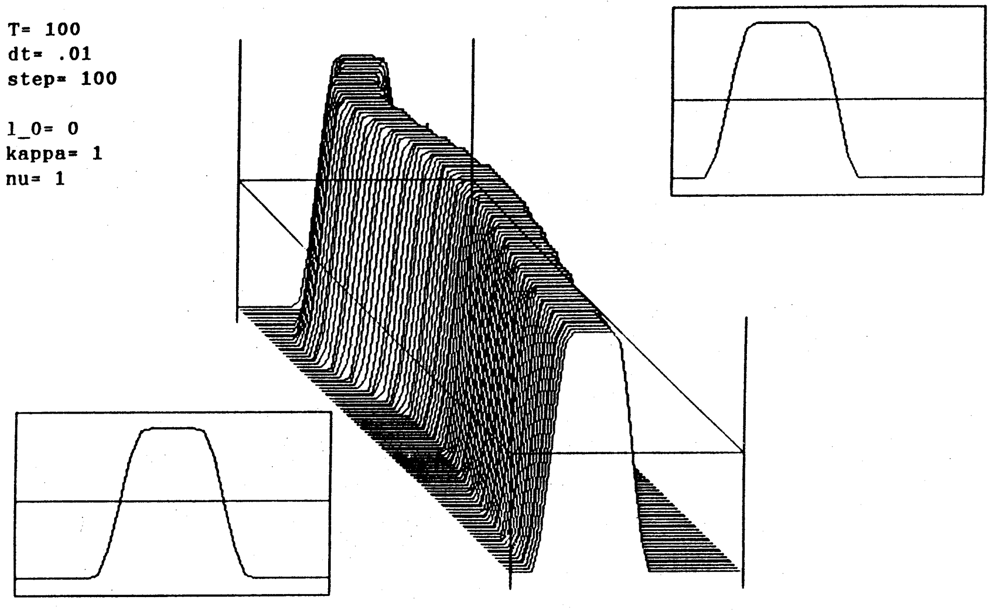
(Fig.3.2)



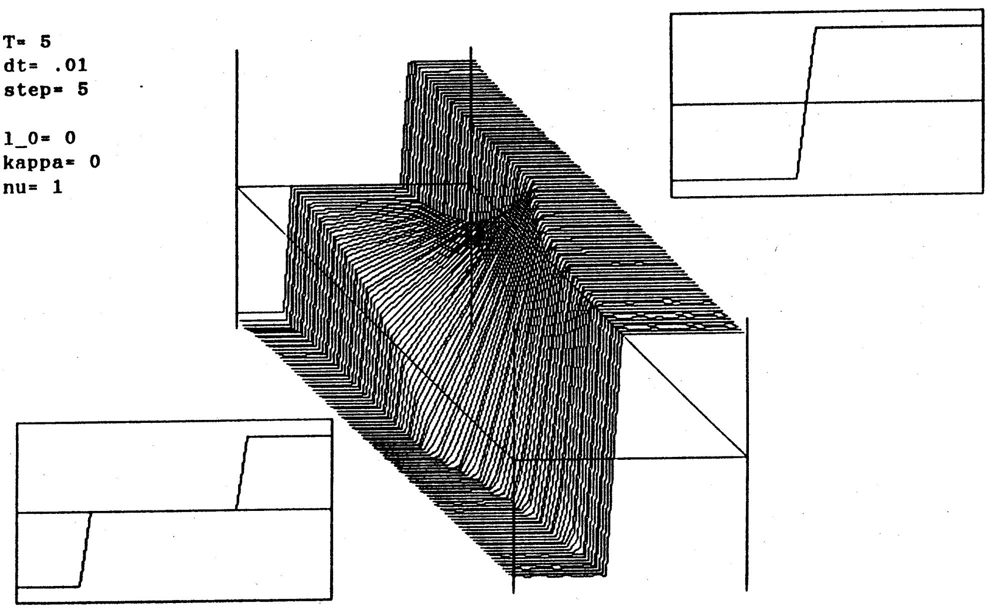
(Fig.3.3)



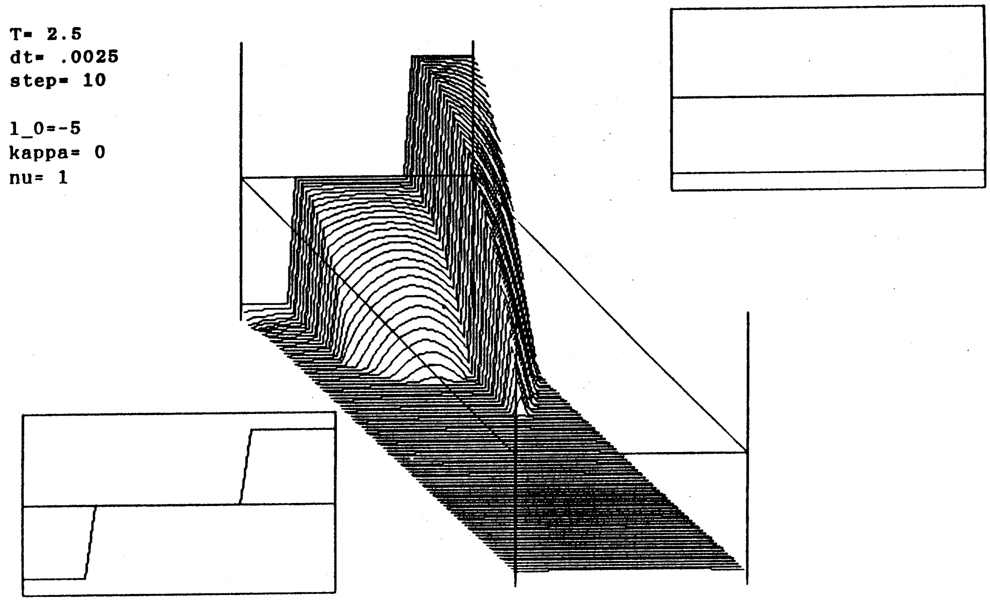
(Fig.3.4)


T= 100
dt= .01
step= 100
l_0= 0
kappa= 1
nu= 1

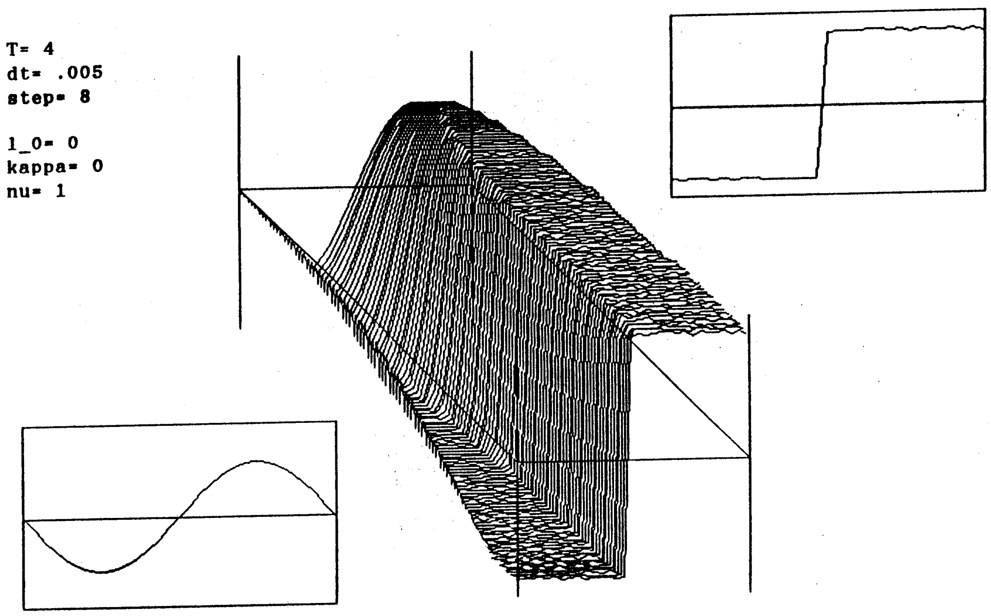
(Fig.3.5)


T= 5
dt= .01
step= 5
l_0= 0
kappa= 0
nu= 1

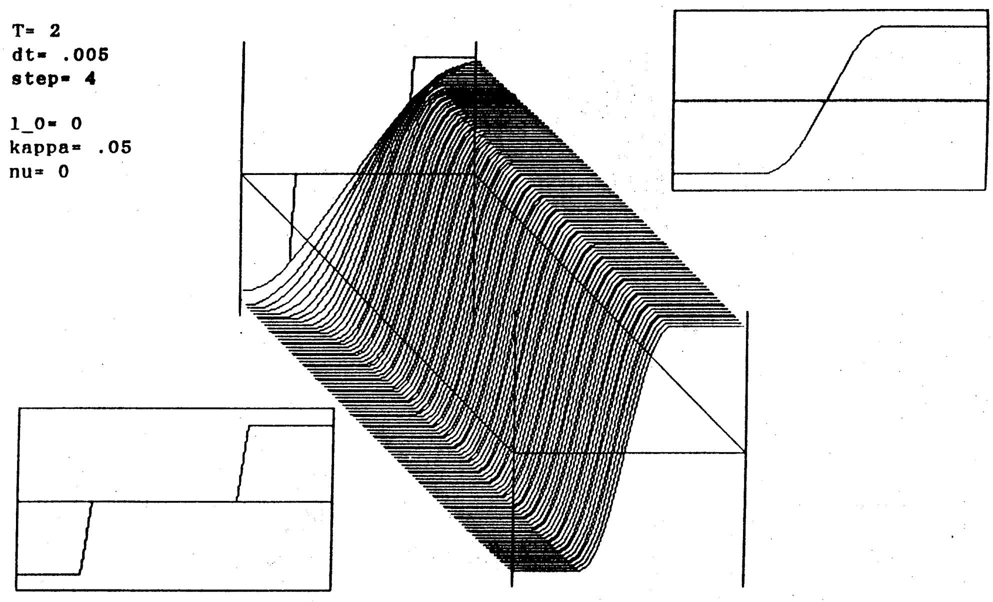
(Fig.3.6)


T= 2.5
dt= .0025
step= 10
l_0=-5
kappa= 0
nu= 1

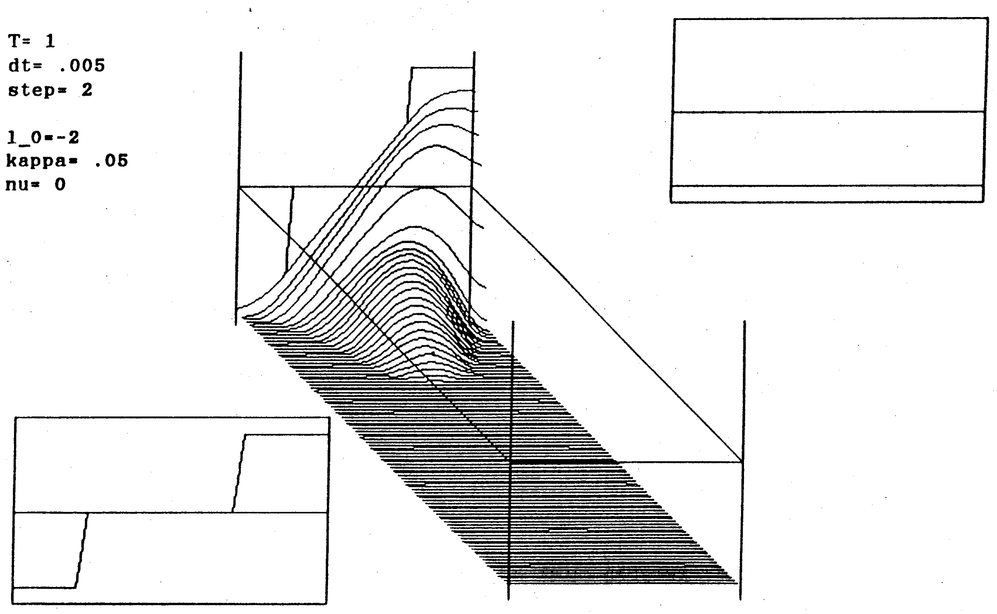
(Fig.3.7)


T= 4
dt= .005
step= 8
l_0= 0
kappa= 0
nu= 1

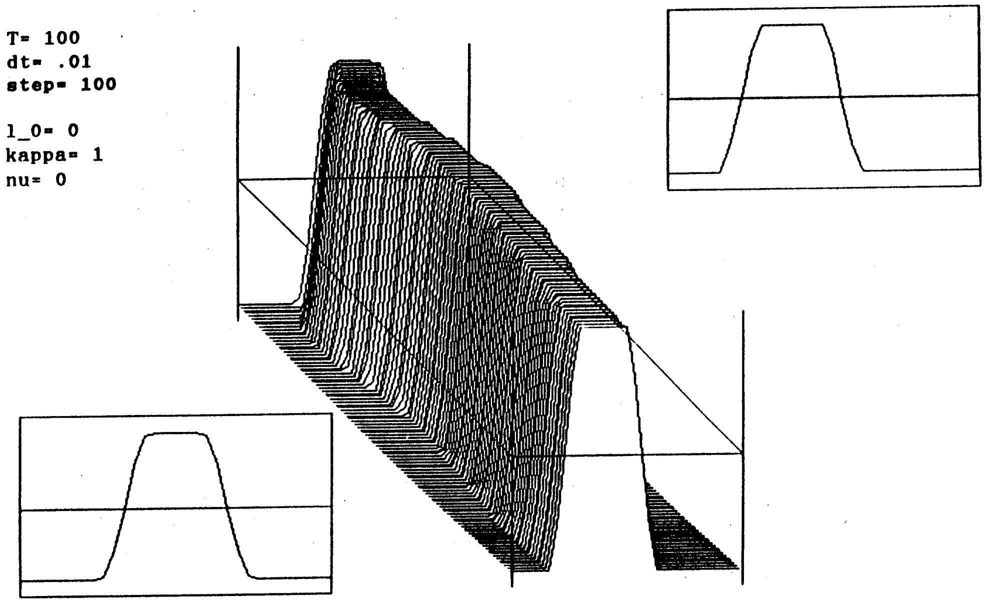
(Fig.3.8)



(Fig.3.9)



(Fig.3.10)



(Fig.3.11)